

## ENHANCED ELLIPTIC GRID GENERATION

### Cross Reference To Related Applications:

This application claims the benefit of U. S. Provisional Application 60/425,750.

### Origin of the Invention:

The invention described herein was made by an employee of the United States Government and may be manufactured and used by or for the Government for governmental purposes without the payment of any royalties thereon or therefor.

### Technical Field:

The present invention is a method for eliminating requirements for parameter inputs for generalized grid generation in modeling of engineering systems.

### Background of the Invention:

A large amount of effort has been devoted to developing, enhancing and using grid generation techniques, through solution of elliptic partial differential equations ("PDEs"). Elliptic grid generation methods generally focus on developing body-conforming grids around bodies for simulations of external fluid flow. The grids thus generated are smooth, having at least continuous first and second derivatives, appropriately stretched or clustered, and are orthogonal over most of the grid domain. Inclusion of inhomogeneous terms in the PDEs allows a grid to satisfy clustering and orthogonality properties in the vicinity of specific surfaces in three dimensions and in the vicinity of specific lines in two dimensions.

Following the work of Thompson, Thames and Mastin, Jour. Computational Physics, vol. 24, 1977, pp. 274-302, three-dimensional governing equations for

elliptic grid generation are often expressed as:

$$\xi_{xx} + \xi_{yy} + \xi_{zz} = P(\xi, \eta, \zeta) = -a_i \operatorname{sgn}(\xi - \xi_i) \exp\{-b_i |\xi - \xi_i|\}, \quad (1A)$$

$$\eta_{xx} + \eta_{yy} + \eta_{zz} = Q(\xi, \eta, \zeta) = -c_i \operatorname{sgn}(\eta - \eta_i) \exp\{-d_i |\eta - \eta_i|\}, \quad (1B)$$

$$\zeta_{xx} + \zeta_{yy} + \zeta_{zz} = R(\xi, \eta, \zeta) = -e_i \operatorname{sgn}(\zeta - \zeta_i) \exp\{-f_i |\zeta - \zeta_i|\}, \quad (1C)$$

where  $\xi$ ,  $\eta$  and  $\zeta$  are generalized curvilinear coordinates,  $x$ ,  $y$  and  $z$  are Cartesian coordinates, and  $P(\xi, \eta, \zeta)$ ,  $Q(\xi, \eta, \zeta)$ , and  $R(\xi, \eta, \zeta)$ , are inhomogeneous terms,  $a_i$ ,  $b_i$ ,  $c_i$ ,  $d_i$ ,  $e_i$  and  $f_i$  are manually selected constants, and the subscript “i” refers to a particular boundary component associated with the problem.

In a two dimensional study by Steger and Sorensen, Jour. Computational Physics, vol. 33, 1979, pp 405-410, the authors use the following governing equations,

$$\xi_{xx} + \xi_{yy} = -a_i \operatorname{sgn}(\eta - \eta_i) \exp\{-d_i |\eta - \eta_i|\}, \quad (1D)$$

$$\eta_{xx} + \eta_{yy} = -c_i \operatorname{sgn}(\eta - \eta_i) \exp\{-d_i |\eta - \eta_i|\}, \quad (1E)$$

for a given  $\eta$  boundary. The quantities  $a_i$  and  $c_i$  are generalized to functions  $a_i(\xi)$  and  $c_i(\xi)$ , respectively, and the values of these quantities are computed as part of the solution by requiring a specified spacing between a given  $\eta$  boundary and an adjacent grid line, and grid orthogonality at this  $\eta$  boundary. In any two dimensional problem, the decay parameters, such as  $d_i$ , must be prescribed or manually inserted for each of the boundaries in any coordinate direction.

However, as will be seen in the subsequent development, these values of  $d_i$  are coupled with the values computed for the quantities  $a_i$  and  $c_i$  respectively so that explicit prescriptions of values for the parameters  $d_i$  are in conflict with the values computed for  $a_i$  and for  $c_i$ . Further, the process of selecting the two values for the parameters  $d_i$  for two opposing boundaries, and, by extension, four values for four boundaries in a two dimensional problem, is cumbersome for static grids and is

infeasible where dynamically changing grids are required. In three dimensions, the parameter values need to be prescribed for six boundaries, one for each of six boundaries.

What is needed is an approach that provides an automatic procedure for generating an elliptic grid that does not require manual insertion or user prescription of these decay parameters for a two dimensional or three dimensional grid generation problem. Preferably, these decay parameters should allow for a variable rate of decay from different points on any grid boundary, should arise automatically in the formulation and solution of the problem and should permit an interpretation in terms of one or more physical quantities associated with the problem.

Summary of the Invention:

These needs are met by the invention, which provides a process for generating an elliptic grid in which (1) grid points tend to cluster near a boundary at a desired rate, which may vary from point to point where one or more coordinate variables may undergo a relatively large change in value), (2) grid lines corresponding to a constant value of a coordinate are approximately parallel to or perpendicular to the local boundary line, and (3) user prescription or manual insertion of parameters to achieve a desired grid behavior in terms of clustering and orthogonality near boundaries is not required (or allowed). The process includes the following steps:

providing defining equations, valid near at least one boundary segment in a generalized coordinate system, of a selected grid system, where each of the defining equations has at least two independent Cartesian coordinate variables, has at least one generalized coordinate as a dependent variable, and comprises a partial differential equation, expressed in at least one generalized coordinate;

providing a selected group of boundary constraints for the grid system, valid near the at least one boundary segment, where a decay parameter for at least one of the generalized coordinate dependent variables near the at least one boundary segment is determined as part of a solution for the grid system, rather than being prescribed initially;

providing defining equations and selected boundary conditions, having at least two independent coordinate variables and at least one dependent variable, for steady state heat transfer on a long thin fin, and providing a correspondence between the at least two independent coordinate variables for the grid system near the at least one grid boundary segment with the at least two independent coordinate variables for the heat transfer problem;

providing a correspondence between a selected power of at least one heat transfer coefficient for the heat transfer problem and at least one decay parameter for the grid system near the at least one grid boundary segment; and

determining a solution of the grid system near the at least one grid boundary segment that incorporates at least one boundary constraint comprising the at least one decay parameter determined for the grid system.

#### Brief Description of the Drawings:

Figure 1 is a flow chart of a procedure for practicing the invention.

Figures 2 and 3 illustrate grids, computed using the invention, for a two dimensional annular region and for a two dimensional convex region, illustrating clustering of grid points near an inner boundary and near an upper boundary, respectively.

### Description of Best Modes of the Invention:

The equations (1A), (1B) and (1C) are modified here in the context of equations (1D) and (1E) and are written in the following form, as a six-equation set for each of the  $(\xi, \eta, \zeta)$  boundaries, where  $a_{k,i} = a_{k,i}(\eta, \zeta)$ ,  $c_{k,i} = c_{k,i}(\xi, \zeta)$ , and  $e_{k,i} = e_{k,i}(\xi, \eta)$  ( $k = 1, 2, 3$ ). The decay parameters  $b_i$ ,  $d_i$  and  $f_i$  are (positive) constants for any given boundary segment and are expressed as parameter functions,  $b_i(\eta, \zeta)$ ,  $d_i(\xi, \zeta)$ , and  $f_i(\xi, \eta)$ . Without loss of generality, one can assume that near a given  $\xi$ -boundary segment  $i$ ,  $\xi - \xi_i \geq 0$ , in a selected region on one side of this boundary segment, where  $\text{sgn}(\xi - \xi_i) > 0$ . Treatment of a situation with  $\text{sgn}(\xi - \xi_i) < 0$  is analogous. In a region close to this boundary segment, where  $b_i(\eta, \zeta)|\xi - \xi_i| \ll 1$ , the defining equations and the nonhomogeneous terms have the forms

$$\xi_{xx} + \xi_{yy} + \xi_{zz} = p_1(\xi, \eta, \zeta), \quad (2A)$$

$$\eta_{xx} + \eta_{yy} + \eta_{zz} = q_1(\xi, \eta, \zeta), \quad (2B)$$

$$\zeta_{xx} + \zeta_{yy} + \zeta_{zz} = r_1(\xi, \eta, \zeta), \quad (2C)$$

$$p_1(\xi, \eta, \zeta) = -a_{1,i}(\eta, \zeta) \text{sgn}(\xi - \xi_i) \exp\{-b_i(\eta, \zeta)|\xi - \xi_i|\}, \quad (2D)$$

$$\approx -a_{1,i}(\eta, \zeta) + a_{1,i}(\eta, \zeta) b_i(\eta, \zeta) (\xi - \xi_i), \quad (2E)$$

$$q_1(\xi, \eta, \zeta) = -c_{1,i}(\eta, \zeta) \text{sgn}(\xi - \xi_i) \exp\{-b_i(\eta, \zeta)|\xi - \xi_i|\}, \quad (2F)$$

$$\approx -c_{1,i}(\eta, \zeta) + c_{1,i}(\eta, \zeta) b_i(\eta, \zeta) (\xi - \xi_i), \quad (2G)$$

$$r_1(\xi, \eta, \zeta) = -e_{1,i}(\eta, \zeta) \text{sgn}(\xi - \xi_i) \exp\{-b_i(\eta, \zeta)|\xi - \xi_i|\}, \quad (2H)$$

$$\approx -e_{1,i}(\eta, \zeta) + e_{1,i}(\eta, \zeta) b_i(\eta, \zeta) (\xi - \xi_i), \quad (2I)$$

In a region close to an  $\eta$ -boundary segment, where  $d_i(\xi, \zeta)|\eta - \eta_i| \ll 1$  and  $\eta - \eta_i \geq 0$ , the defining equations and the nonhomogeneous terms have the forms

$$\xi_{xx} + \xi_{yy} + \xi_{zz} = p_2(\xi, \eta, \zeta), \quad (3A)$$

$$\eta_{xx} + \eta_{yy} + \eta_{zz} = q_2(\xi, \eta, \zeta), \quad (3B)$$

$$\zeta_{xx} + \zeta_{yy} + \zeta_{zz} = r_2(\xi, \eta, \zeta), \quad (3C)$$

$$p_2(\xi, \eta, \zeta) = -a_{2,i}(\xi, \zeta) \operatorname{sgn}(\eta - \eta_i) \exp\{-d_i(\xi, \zeta)|\eta - \eta_i|\}, \quad (3D)$$

$$\approx -a_{2,i}(\xi, \zeta) + a_{2,i}(\xi, \zeta) d_i(\xi, \zeta) (\eta - \eta_i), \quad (3E)$$

$$q_2(\xi, \eta, \zeta) = -c_{2,i}(\xi, \zeta) \operatorname{sgn}(\eta - \eta_i) \exp\{-d_i(\xi, \zeta)|\eta - \eta_i|\}, \quad (3F)$$

$$\approx -c_{2,i}(\xi, \zeta) + c_{2,i}(\xi, \zeta) d_i(\xi, \zeta) (\eta - \eta_i), \quad (3G)$$

$$r_2(\xi, \eta, \zeta) = -e_{2,i}(\xi, \zeta) \operatorname{sgn}(\eta - \eta_i) \exp\{-d_i(\xi, \zeta)|\eta - \eta_i|\}, \quad (3H)$$

$$\approx -e_{2,i}(\xi, \zeta) + e_{2,i}(\xi, \zeta) d_i(\xi, \zeta) (\eta - \eta_i), \quad (3I)$$

In a region close to an  $\zeta$ -boundary segment, where  $f_i(\xi, \eta) |\zeta - \zeta_i| \ll 1$  and  $\zeta - \zeta_i \geq 0$ , the defining equations and the nonhomogeneous terms have the forms

$$\xi_{xx} + \xi_{yy} + \xi_{zz} = p_3(\xi, \eta, \zeta), \quad (4A)$$

$$\eta_{xx} + \eta_{yy} + \eta_{zz} = q_3(\xi, \eta, \zeta), \quad (4B)$$

$$\zeta_{xx} + \zeta_{yy} + \zeta_{zz} = r_3(\xi, \eta, \zeta), \quad (4C)$$

$$p_3(\xi, \eta, \zeta) = -a_{3,i}(\xi, \eta) \operatorname{sgn}(\zeta - \zeta_i) \exp\{-f_i(\xi, \eta)|\zeta - \zeta_i|\}, \quad (4D)$$

$$\approx -a_{3,i}(\xi, \eta) + a_{3,i}(\xi, \eta) f_i(\xi, \eta) (\zeta - \zeta_i), \quad (4E)$$

$$q_3(\xi, \eta, \zeta) = -c_{3,i}(\xi, \eta) \operatorname{sgn}(\zeta - \zeta_i) \exp\{-f_i(\xi, \eta)|\zeta - \zeta_i|\}, \quad (4F)$$

$$\approx -c_{3,i}(\xi, \eta) + c_{3,i}(\xi, \eta) f_i(\xi, \eta) (\zeta - \zeta_i), \quad (4G)$$

$$r_3(\xi, \eta, \zeta) = -e_{3,i}(\xi, \eta) \operatorname{sgn}(\zeta - \zeta_i) \exp\{-f_i(\xi, \eta)|\zeta - \zeta_i|\}, \quad (4H)$$

$$\approx -e_{3,i}(\xi, \eta) + e_{3,i}(\xi, \eta) f_i(\xi, \eta) (\zeta - \zeta_i), \quad (4I)$$

Where the preceding approximations, near a boundary segment  $\zeta = \zeta_i$ , for example, are used, the defining equations for  $\zeta$  become

$$\xi_{xx} + \xi_{yy} + \xi_{zz} - a_{3,i}(\xi, \eta) f_i(\xi, \eta) (\zeta - \zeta_i) = -a_{3,i}(\xi, \eta) \operatorname{sgn}(\zeta - \zeta_i), \quad (5A)$$

$$\eta_{xx} + \eta_{yy} + \eta_{zz} - c_{3,i}(\xi, \eta) f_i(\xi, \eta) (\zeta - \zeta_i) = -c_{3,i}(\xi, \eta) \operatorname{sgn}(\zeta - \zeta_i), \quad (5B)$$

$$\zeta_{xx} + \zeta_{yy} + \zeta_{zz} - e_{3,i}(\xi, \eta) f_i(\xi, \eta) (\zeta - \zeta_i) = -e_{3,i}(\xi, \eta) \operatorname{sgn}(\zeta - \zeta_i). \quad (5C)$$

If one ignores the nonhomogeneous terms on the right hand side of Eq. (5C) and ignores the dependence upon  $z$  (or  $\zeta$ ), this relation is seen to represent a steady

state heat transfer equation for a long, thin fin of width or height  $2L$ , with corresponding “temperature”  $\theta = \xi - \xi_I$ , discussed, for example, by V. S. Arpaci in Conduction Heat Transfer, Addison Wesley, Reading, Mass., 1966, pp. 145-147 and 201-205:

$$\partial^2\theta/\partial x^2 + \partial^2\theta/\partial y^2 - m^2 \theta = 0, \quad (6)$$

$$m^2 = 2h/k\delta. \quad (7)$$

where  $h$  is a heat transfer coefficient in a selected ( $z$ -) direction,  $k$  is a thermal conductivity coefficient and  $\delta$  ( $\ll L$ ) is thickness of the fin. Similar equations apply for  $\theta = \xi - \xi_I$ , and  $\theta = \eta - \eta_I$ .

The heat transfer coefficient  $h$  corresponds to or is proportional to, for example, a decay parameter, such as the coefficient  $e_{3,i}(\xi, \eta)f_i(\xi, \eta)$  in Eq. (4I). Similar equations are developed for the choices  $\theta = \xi - \xi_I$ , or  $\theta = \eta - \eta_I$ .

Where the heat transfer coefficient  $h$  in the  $z$ -direction is small, the thermal gradient is correspondingly large normal to the corresponding boundary in the  $xy$ -space, which requires a close clustering of isothermal lines, or of the corresponding time evolving grid lines. This provides a physical basis for the observation that clustering near a given boundary increases as a decay parameter (e.g.,  $m^2$  in Eq. (7)) decreases, and inversely. However, for a grid whose grid lines show a general dependence upon both coordinates,  $x$  and  $y$  (as in Figures 2 and 3, discussed in the following), a similar conclusion is arrived at using the following physical argument. As the heat transfer coefficient  $h$  in the  $z$ -direction decreases, the temperature gradient near a  $y$ -boundary increases correspondingly, for a given heat flux, and this leads to a denser clustering of isothermal lines (or, equivalently, of grid lines for the time evolving grid).

Boundary constraints, valid in a one-sided neighborhood of each of the four (two dimensional) or six (three dimensional) boundary segments, are incorporated

by applying Green's theorem in three dimensions for each of the Eqs. (2E), (3G) and (4I) for the  $\xi$ ,  $\eta$  and  $\zeta$  boundaries, respectively:

$$\int_S (\partial\theta/\partial n) d\sigma = \int_V \{-a_{1,i}(\eta, \zeta) \operatorname{sgn}(\xi - \xi_i) + a_{1,i}(\eta, \zeta) b_i(\eta, \zeta) \theta\} d\tau, \quad (8)$$

$$\int_S (\partial\theta/\partial n) d\sigma = \int_V \{-c_{2,i}(\xi, \zeta) \operatorname{sgn}(\eta - \eta_i) + c_{2,i}(\xi, \zeta) d_i(\xi, \zeta) \theta\} d\tau, \quad (9)$$

$$\int_S (\partial\theta/\partial n) d\sigma = \int_V \{-e_{3,i}(\xi, \eta) \operatorname{sgn}(\zeta - \zeta_i) + e_{3,i}(\xi, \eta) f_i(\xi, \eta) \theta\} d\tau, \quad (10)$$

where  $n$  refers to a direction that is locally normal to a surface  $S$  representing a totality of six surfaces including the boundary segments of interest and  $V$  is a volume enclosed or defined by the totality of these six surfaces. These integral-type boundary constraints can be used to calculate the decay parameter analogs,  $a_{1,i}(\eta, \zeta)b_i(\eta, \zeta)$ ,  $c_{2,i}(\eta, \zeta)d_i(\xi, \zeta)$  and  $e_{3,i}(\eta, \zeta)f_i(\xi, \eta)$ . When expressed in terms of the generalized coordinates  $(\xi, \eta, \zeta)$ , the boundary constraints set forth in Eqs. (8), (9) and (10) are transformed, for  $\zeta$  for example, as follows.

$$\int_S I d\sigma = \int_S (\partial\theta/\partial n) d\sigma = \int_S (\partial\zeta/\partial n) d\sigma \quad (11)$$

The integral  $\int_S I d\sigma$  in Eq. (14) can be written as an algebraic sum of six integrals, evaluated over the indicated boundary segments:

$$\begin{aligned} \int_S I d\sigma = & \int_{\xi_{\max}} I d\sigma + \int_{\eta_{\max}} I d\sigma + \int_{\zeta_{\max}} I d\sigma \\ & - \int_{\xi_{\min}} I d\sigma - \int_{\eta_{\min}} I d\sigma - \int_{\zeta_{\min}} I d\sigma, \end{aligned} \quad (12)$$

where the surface configurations  $\xi_{\max}$ ,  $\xi_{\min}$ , etc. represent the corresponding boundary segments that together make up the surface  $S$ . For the first and fourth integral pair, the second and fifth integral pair, and the third and sixth integral pair in Eq. (15), the following respective relations may be verified:

$$\int_{\xi} I d\sigma = \int_{\xi} (1/J\sqrt{\alpha_{11}}) \alpha_{13} [(\eta^2 + y_{\eta}^2 + z_{\eta}^2)(x_{\xi}^2 + y_{\eta}^2 + z_{\xi}^2)]^{1/2} d\zeta d\eta. \quad (13)$$

$$\begin{aligned} \int_{\eta} I d\sigma = & \int_{\eta} (1/J\sqrt{\alpha_{22}}) \alpha_{23} [(x_{\xi}^2 + y_{\xi}^2 + z_{\eta}^2)(x_{\xi}^2 + y_{\xi}^2 \\ & + z_{\xi}^2)]^{1/2} d\xi d\zeta, \end{aligned} \quad (14)$$

$$\int_{\zeta} I d\sigma = \int_{\zeta} (1/J) [\alpha_{33} (x_{\eta}^2 + y_{\eta}^2 + z_{\eta}^2)(x_{\xi}^2 + y_{\xi}^2 + z_{\xi}^2)]^{1/2} d\eta d\xi, \quad (15)$$



$$\alpha_{11} = J^2(\xi_x^2 + \xi_y^2 + \xi_z^2), \quad (16A)$$

$$\alpha_{22} = J^2(\eta_x^2 + \eta_y^2 + \eta_z^2), \quad (16B)$$

$$\alpha_{33} = J^2(\zeta_x^2 + \zeta_y^2 + \zeta_z^2), \quad (16C)$$

$$\alpha_{12} = J^2(\xi_x \eta_x + \xi_y \eta_y + \xi_z \eta_z), \quad (16D)$$

$$\alpha_{13} = J^2(\xi_x \zeta_x + \xi_y \zeta_y + \xi_z \zeta_z), \quad (16E)$$

$$\alpha_{23} = J^2(\eta_x \zeta_x + \eta_y \zeta_y + \eta_z \zeta_z), \quad (16F)$$

where  $J = J((x,y,z)/(\xi,\eta,\zeta))$  is a Jacobian of the transformation  $(x,y,z) \rightarrow (\xi,\eta,\zeta)$ .

Equations (13)-(15) can be used to express the boundary constraints in the computational space (generalized variables  $(\xi,\eta,\zeta)$ ), analogous to the Eqs. (8)-(10) expressed in Cartesian coordinate space. The defining equations in computational space that are solved, subject to the boundary constraints set forth in Eq. (4I) for a  $\zeta$ -boundary, are

$$\begin{aligned} \alpha_{11} x_{i,\xi\xi} + \alpha_{22} x_{i,\eta\eta} + \alpha_{33} x_{i,\zeta\zeta} + 2\{\alpha_{12} x_{i,\xi\eta} + \alpha_{13} x_{i,\xi\zeta} + \alpha_{23} x_{i,\eta\zeta}\} = \\ = -J^2\{p_3 x_{i,\xi} + q_3 x_{i,\eta} + r_3 x_{i,\zeta}\}, \end{aligned} \quad (17)$$

$$x_i = x, y \text{ or } z. \quad (18)$$

Figure 1 is a flow chart of a suitable procedure for practicing the invention for a two dimensional or three dimensional grid system. In step 11, the system provides defining equations, valid near one or more grid boundary segments in a generalized coordinate system, of a selected grid system, where each of the defining equations has at least two independent Cartesian coordinate variables, has at one generalized coordinate as a dependent variable, and comprises a partial differential equation, expressed in at least one generalized coordinate.

In step 13, the system provides a selected group of boundary constraints for the grid system, valid near the one or more boundary segments, where a decay parameter for at least one of the generalized coordinate dependent variables near

the one or more boundary segments is determined as part of a solution of the defining equations, rather than being prescribed initially.

In step 15, the system provides defining equations and selected boundary conditions, having at least two independent coordinate variables, for steady state heat transfer on a long thin fin, and the system provides a correspondence between the at least two independent coordinate variables for the grid system near at least one grid boundary segment with the at least two independent coordinate variables for the heat transfer problem.

In step 17, the system provides a correspondence a selected power of at least one heat transfer coefficient for the heat transfer problem and at least one decay parameter for the grid system near the at least one grid boundary segment.

In step 19, the system determines a solution of the grid system near the at least one grid boundary segment that incorporates at least one boundary constraint comprising the at least one decay parameter determined for the grid system.

Figure 2 illustrates a result of application of the invention to a two dimensional annular region to provide a grid in which grid points cluster near an inner boundary of the annulus. Where a geometrical system, such as an annulus, evolves with time, a grid according to the invention is developed at each of a selected sequence of times, with the parameters subject to the boundary constraints being allowed to vary from one time to another time. Each of these grids can be used to perform a finite element or finite difference analysis on the geometrical object that represents the time evolving system at one of these times.

Figure 3 illustrates a result of application of the invention to a two dimensional convex-concave geometry region to provide a grid in which grid points cluster near an upper boundary of the region.

A decay parameter, such as  $e_{3,i}(\xi,\eta)f_i(\xi,\eta)$ , may vary with one or more of the generalized coordinates, such as  $\xi$  and/or  $\eta$ , rather than being constant; and this variation is determined as part of the solution of the grid problem, rather than being prescribed initially by the user. A grid solution can be determined for a temporally constant environment. Alternatively, a time evolving environment can be allowed to vary at each of a sequence of times, and a grid solution can be determined for each of this sequence of times, using the preceding analysis at each of these times.

The preceding analysis has focused on neighborhoods of the grid boundary segments. As noted in the preceding, in an interior region, far from the grid boundary segments, the defining partial differential equations (PDEs) become homogeneous, and standard analysis of elliptic PDEs is applied to determine an interior solution, which is automatically matched in the solution process across a selected interior boundary to the solution obtained for the grid boundary segments.